

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:** 2.19e-15 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:** 2.47e-01

**Confidence level:** 4.80e-01

## Nearest Neighbors from the Training Set

Image not found

Perfluorotributylamine

**Measured:** 6.00e-17

**Predicted:** 1.14e-16

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Butane, 1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxy-

**Measured:** 7.20e-15

**Predicted:** 1.32e-14

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Perfluorotriethylamine

**Measured:** 6.00e-16

**Predicted:** 6.45e-16

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1-Butanol, 2,2,3,3,4,4,4-heptafluoro-

**Measured:** 1.12e-13

**Predicted:** 6.54e-14